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ELASTIC SCATTERING OF ZERO ENERGY POSITRONS BY HELIUM ATOMS

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October 1969

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ELASTIC SCATTERING OF ZERO ENERGY POSITRONS BY HELIUM ATOMS

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ABSTRACT

Kohn's variational method is used to calculate the scattering length for collisions between zero energy positrons and helium atoms in their ground state. The trial function used depends on several exponential parameters and up to twenty linear parameters and includes explicitly correlation between the positron and the electrons of the atom. The trial function also depends on the ground state wave function ψ_0 of the helium atom and we have attempted calculations using six different approximations to ψ_0 . The calculations all seem to diverge except when a Hartree Fork approximation to ψ_0 is used, although with a three term Hylleraas ψ_0 we get the value $-0.592a_0$ for the scattering length.

We have also calculated the effective electron number Z_{eff} which gives the rate of annihilation of positrons in helium. An error in a previous paper by Houston (1968) is corrected.

ELASTIC SCATTERING OF ZERO ENERGY POSITRONS BY HELIUM ATOMS

1. Introduction

In a recent paper, Houston and Moiseiwitsch (1968) have calculated the scattering length for elastic collisions between zero energy positrons and helium atoms using Kohn's variational method. The trial scattering wave function used allowed explicitly for correlation between the incident positron and the target electrons. It contained up to twenty linear parameters and three adjustable exponential parameters. However the representation used for the helium atom ground state wave function was the analytic Hartree-Fock wave function of Green et al. (1954) and this did not allow explicitly for correlation between the atomic electrons. It is the purpose of the present paper to investigate the use of different helium atom ground state wave functions, which allow for interelectronic correlation in varying degrees, in a variational calculation of the scattering length.

Now it is well known that Kohn's variational method gives an upper bound to the scattering length when there are no composite bound states of the incident particle and the target atom (Spruch and Rosenberg, 1960), provided that the exact target wave function is used. We cannot of course do this for helium, but we have shown below that Kohn's variational method in this case should still yield a good approximation to the scattering length, which will probably be an upper bound, provided that the helium ground state wave function used is fairly accurate.

Calculations of the scattering length for elastic collisions between positrons and helium atoms have also been performed by Kestner et al. (1965) using a pseudopotential model, by Hashino (1966) using the method of polarized orbitals and by Drachman (1968) who has used a first order adiabatic correlation trial function in both variational and non-variational calculations.

In addition to the scattering length calculations, the positron annihilation rate in helium has been calculated using the scattering wave functions obtained in two of the different cases examined. These values are compared with recent theoretical and experimental results.

2. Variational Method

We want to derive Kohn's variational principle for the scattering length for the case where the helium atom ground state wave function has been derived using the variational principle for bound states.

Let us suppose that ψ_0 denotes the exact ground state wave function of the target atom, having exact eigenergy E_0, and that the trial scattering wave function Ψ_T for the entire system has the asymptotic form

$$\Psi_T \sim \frac{a_T - r_1}{r_1} \psi_0 \qquad (1)$$

for large radial distances r_1, of the incident positron from the atomic nucleus. a_T is an adjustable parameter representing the scattering length. Then Kohn's variational approximation to the scattering length is

$$a_v = a_T + \frac{1}{4\pi}\frac{2m}{\hbar^2}\int \Psi_T(H - E_0)\Psi_T d\tau \tag{2}$$

where H is the total Hamiltonian for the whole system and the integration is over all the spatial coordinates of the positron and atomic electrons. The trial scattering function Ψ_T will contain a_T and probably other adjustable parameters $c_i (i = 1, .n)$, and the optimum values of these parameters are obtained from the n + 1 Kohn variational equations

$$\frac{\partial a_v}{\partial a_T} = 0, \frac{\partial a_v}{\partial c_i} = 0 \ (i = 1, ..n) \tag{3}$$

Furthermore, since there are no composite bound states of the system of positron and helium atom (Gertler et al., 1968) we have

$$a \leq a_v \tag{4}$$

where a is the exact scattering length (Spruch and Rosenberg , 1960).

Let us now consider the case where the target ground state wave function and energy are determined using the Rayleigh-Ritz variational method for bound states.

Suppose Ψ is the exact scattering wave function for zero energy positrons off helium atoms. Then the integral

$$I \int \psi(H - E_0)\psi \, d\tau = 0 \tag{5}$$

where the integration is as in (2) above. Now ψ has the asymptotic form

$$\psi \sim \frac{a - r_1}{r_1} \psi_0 \tag{6}$$

as $r_1 \to \infty$, and so a small change in ψ has the asymptotic form

$$\delta\psi \sim \frac{1}{r_1} \delta(a\psi_0) = \delta\psi_0 \tag{7}$$

Also if H_0 is the Hamiltonian for the helium atom, then

$$E_0 = \int \psi_0 H_0 \psi_0 \, d\tau' \tag{8}$$

where the integration is over the spatial coordinates of the atomic electrons only. Now the Rayleigh-Ritz theorem tells us that a first order change in ψ_0 produces a second order change in E_0 , that is, since

$$\delta E_0 = 0 \tag{9}$$

we have

$$\int \delta\psi_0 H_0 \delta\psi_0 \, d\tau = \delta^2 E_0 \tag{10}$$

where $\delta^2 E_0$ is of the second order of smallness.

Now let us consider small variations in I caused by changes in Ψ . We have

$$\delta I = \int (\Psi + \delta\Psi)(H - E_0 - \delta^2 E_0)(\Psi + \delta\Psi) d\tau$$

$$- \int \Psi (H - E_0) \Psi \, d\tau \tag{11}$$

We are supposing that $(\Psi + \delta\Psi)$ contains an approximation to ψ_0 which has been obtained using the Rayleigh-Ritz theorem, and so we must include the small change in the energy.

Expanding (11) we have

$$\delta I = \int \delta\Psi (H - E_0) \Psi \, d\tau + \int \Psi (H - E_0) \delta\Psi \, d\tau$$

$$+ \int \delta\Psi (H - E_0) \delta\Psi \, d\tau - \delta^2 E_0 \int (\Psi + \delta\Psi)^2 \, d\tau. \tag{12}$$

The last term is an addition to the usual Kohn expression which is derived assuming that ψ_0 and E_0 are exact.

Now, using Green's theorem, we have

$$\int \Psi (H - E_0) \delta\Psi \, d\tau$$

$$= \int \delta\Psi (H - E_0) \Psi \, d\tau \qquad (13)$$

$$+ \frac{\hbar^2}{2m} \int \left(\delta\Psi \frac{\partial\Psi}{\partial n_1} - \Psi \frac{\partial(\delta\Psi)}{\partial n_1} \right) dS_1 \, d\tau'$$

where the integration dS_1, is over a large sphere in r_1 space, n_1, being a unit vector normal to this sphere.

When we insert the asymptotic forms (6) and (7) of Ψ and $\delta\Psi$, the right hand side of (13) becomes

$$\int \delta\Psi (H - E_0) \Psi \, d\tau - 4\pi \frac{\hbar^2}{2m} \delta a \left\{ 1 + \int \psi_0 \delta\psi_0 \, d\tau \right\} \qquad (14)$$

Now

$$(H - E_0)\Psi = 0 \qquad (15)$$

since Ψ is an exact solution, and

$$\int \psi_0^2 \, d\tau' = 1 \qquad (16)$$

so we can write

$$\delta I = -4\pi \frac{\hbar^2}{2m} \delta a \int \psi_0 \, (\psi_0 + \delta\psi_0) \, d\tau'$$
$$+ \int \delta\Psi (H - E_0) \, \delta\Psi d\tau - \delta^2 E_0 \int (\Psi + \delta\Psi)^2 \, d\tau . \tag{17}$$

If we let

$$\chi_T = \chi + \delta\chi \tag{18}$$

for $\chi = \Psi \; , \psi_0 \; , E_0$ and a, in turn, we have

$$a = a_T + \frac{1}{4\pi} \frac{2m}{\hbar^2} \cdot \frac{1}{\Delta} \left[\int \Psi_T \, (H - E_{0T}) \Psi_T \, d\tau \right.$$
$$\left. - \int \delta\Psi (H - E_0) \, \delta\Psi \, d\tau + \delta^2 E_0 \int \Psi_T^2 \, d\tau \right] \tag{19}$$

where

$$\Delta = \int \psi_0 \, \psi_{0T} \, d\tau' \; . \tag{20}$$

If we neglect the second order terms (to this order $\Delta = 1$) then we have the usual Kohn variational approximation a_v as given by (2).

The first of the second order terms

$$\int \delta\Psi\,(H - E_0)\,\delta\Psi\,d\tau \tag{21}$$

is a positive definite (or zero) number and if the other second order term were not there, then the neglect of (21) would lead to the upper bound $a \leq a_v$. But the integral in the second term

$$\delta^2 E_0 \int \Psi_T^2\, d\tau \tag{22}$$

is infinite and so we may not even get a good approximation to a. However, we can show that for large r_1, the two second order terms cancel out.

$$\begin{aligned} &- \int \delta\Psi\,(H - E_0)\,\delta\Psi\,d\tau + \delta^2 E_0 \int (\Psi + \delta\Psi)^2\, d\tau \\ &\sim - \int \left(\frac{a + \delta a - r_1}{r_1}\right)^2 d\tau_1 \int \delta\psi_0\,(H_0 - E_0)\;\delta\psi_0\, d\tau' \\ &+ \int \delta\psi_0 H_0\, \delta\psi_0\, d\tau' \int \left(\frac{a + \delta a - r_1}{r_1}\right)^2 d\tau_1 \end{aligned}$$

as $r_1 \to \infty$

$$= E_0 \int \left(\frac{a + \delta a - r_1}{r_1}\right)^2 d\tau_1 \int (\delta\psi_0)^2 d\tau' \tag{23}$$

where the integration $d\tau$, is over the coordinates of the positron and $d\tau = d\tau_1 d\tau'$. Now we can choose $(\psi_0 + \delta\psi_0)$ such that

$$\int (\psi_0 + \delta\psi_0)^2\, d\tau' = 1 \tag{24}$$

and, using (16), we have

$$2 \int \psi_0 \delta\psi_0 d\tau' + \int (\delta\psi_0)^2 d\tau' = 0 \qquad (25)$$

Now

$$E_0 = \int \psi_0 H_0 \psi_0 d\tau'$$

and so

$$\delta^2 E_0 = \int (\psi_0 + \delta\psi_0) H_0 (\psi_0 + \delta\psi_0) d\tau' - \int \psi_0 H_0 \psi_0 d\tau'$$

$$= 2 E_0 \int \psi_0 \delta\psi_0 d\tau' + \delta^2 E_0$$

giving

$$\int \psi_0 \delta\psi_0 d\tau' = 0 \qquad (26)$$

Hence for large r_1 the second order terms in the variational approximation (19) cancel out.

This implies that for most good choices of ψ_0 we shall get a good approximation to the exact scattering length.

3. Details of the wave function

The trial scattering wave functions used were similar to that used by Houston and Moiseiwitsch (1968) and were of the form

$$\Psi_T(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \phi(r_1, r_2, r_{12}, r_3, r_{13})\psi_{0T}(\mathbf{r}_2, \mathbf{r}_3) \qquad (27)$$

where the suffix 1 refers to the positron, and 2 and 3 to the atomic electrons. ϕ is given by

$$\phi(r_1, r_2, r_{12}, r_3, r_{13}) = \frac{a_T(1 - e^{-\delta r_1}) - r_1}{r_1}$$

$$+ e^{-\alpha r_1} \sum_{i=1}^{S} a_i \left\{ e^{-\beta r_2} \chi_i(r_1, r_2, r_{12}) \right.$$

$$\left. + e^{-\beta r_3} \chi_i(r_1, r_3, r_{13}) \right\} \qquad (28)$$

where

$$\chi_i(r_1, r_2, r_{12}) = r_1^{\ell} r_2^{m} r_{12}^{n} \quad (\ell, m, n, \geq 0). \qquad (29)$$

Our calculations were performed for S = 4, 10, and, in several cases, 20, corresponding to the inclusion of all terms satisfying $\ell, m, n, \leq 1, 2, 3$, respectively.

$\psi_{0T}(\mathbf{r}_2, \mathbf{r}_3)$ is the ground state wave function for the helium atom and we used the following six approximations:

I 1 term Hylleraas $N e^{-z_1 s}$ (30a)

II 2 term Hylleraas $N e^{-z_1 s}(1 + c_1 u)$ (30b)

III 3 term Hylleraas $N e^{-z_1 s}(1 + c_1 u + c_2 t^2)$ (30c)

where $s = r_2 + r_3$, $t = r_2 - r_3$, $u = r_{23}$.

IV Hartree-Fock $N \left(e^{-z_1 r_1} + c_1 e^{-z_2 r_1}\right) \left(e^{-z_1 r_2} + c_1 e^{-z_2 r_2}\right)$ (30d)

V Modified Hartree-Fock $N \left(e^{-z_1 r_1} + c_1 e^{-z_2 r_1}\right) \left(e^{-z_1 r_2} + c_1 e^{-z_2 r_2}\right)$
$\times (1 + c_2 r_{23})$ (30e)

VI Hylleraas-Eckart $N \left(e^{-z_1 r_1 - z_2 r_2} + e^{-z_2 r_1 - z_1 r_2}\right)$ (30f)

The details of these six wave functions are given in Table I.

Also given in Table I are the ground state energies E_{0T} obtained with these wave functions, and values of

$$\Delta = \int \psi_0 \, \psi_{0T} \, d\tau'$$

where ψ_{0T} is the trial ground state wave function and ψ_0 is the twenty term ground state wave function of Hart and Herzberg (1957). This ψ_0 is so much more exact than any of the above six that the values of Δ given in Table I are a very good approximation to the Δ defined by equation (20).

4. Scattering Results

Table II gives the values of the variational approximations to the scattering length obtained using the approximations (30) to ψ_0 in conjunction with (27). Table III gives the values of the exponential parameters δ, α, β appropriate to each case.

When the very simple Hylleraas ground state wave function I was used, the minimum value of 0.061 a_0 was obtained for the scattering length with $S = 4$ for the values of δ and α given. The parameter β was fixed at 0.0 because it was found that the calculation was unstable for non-zero values of β, giving large negative values for a_v. With the same values of δ, α and β, S was increased to 10 and this resulted in the value $-8.397a_0$ for a_v. This is obviously too large in absolute value and so we conclude that wave function I is inadequate for this type of variational calculation. It is worth noting that the value of Δ for this wave function is the worst of the six values obtained.

In the two term Hylleraas wave function, II, we picked the same values of δ, α and β that were "best" for I and we noted a similar behaviour in the values obtained for a_v. There is a marked improvement in the value obtained with $S = 10$, but it is still too large and negative even though a considerably better value for Δ is obtained.

However with the three term Hylleraas wave function, III, we have obtained our "best" overall value for the scattering length. The values of δ, α and β were those which gave the best value for a_v at the $S = 4$ stage. This was $-0.186a_0$ and when S was increased to 20, keeping the same values for δ, α and β, we obtained $-0.592a_0$ for the scattering length. However, as can be seen

from Table II, it is not obvious that a_v is converging for this trial function as S is increased and so it may happen that a_v will become large and negative after a few more terms, as happened for functions I and II. Nevertheless this value of $-0.592a_0$ is in good agreement with those calculated by Drachman (1968) who gets $-0.659a_0$ using a non-variational method and $-0.511a_0$ using a variational bound method, with Kestner et al. (1965) who get $-0.575a_0$, and with Hashino (1966) who obtained $-0.546a_0$. It is worth noting that the value obtained for Δ with wave function III is the best we have calculated and only differs from unity by 10^{-4}.

The results for the Hartree Fock wave function, IV, have been reported previously (Houston and Moiseiwitsch, 1968). In this case the values of δ, α and β are those which are "best" for S = 10. Furthermore as S is increased, the values for the scattering length seem to be converging. In the case of the Modified Hartree Fock wave function, V, we only calculated one value for a_v, using the same values for δ, α and β as were used for wave function IV. Furthermore we only took S = 10. The value obtained for a_v was not as good as the corresponding value obtained using the Hartree Fock function and so this choice for the exponential parameters was a very poor one. Had we optimized these, we should have gotten an improvement over IV. However this calculation took a long time and we did not proceed with it.

Finally the Hylleraas Eckart wave function VI produced values for a_v which were disappointing in that they seemed to be converging until S was about 17 when they suddenly became large and negative, in a similar way to I and II, although not to such an extent. In this case it was also found that the parameter

could not be varied from 0.0 and the values for δ and σ are those which were "best" for S = 4.

So it seems that with the type of scattering wave functions given by (27), the only reliable form for η_{0T} is IV, the Hartree Fock representation. Certainly a better value for the scattering length is obtained using the three term Hylleraas wave function III, but it is not clear that the values obtained are converging with increasing S as they seem to be doing when wave function IV is used.

5. Positron Annihilation

The rate of annihilation of positrons in helium gas is given by the expression

$$\Lambda = \pi r_0^2 \, c N_a \, Z_{eff}$$

(Ferell, 1956) where r_0 is the classical electron radius e^2/mc^2, N_a is the number density of atoms in the target gas and Z_{eff} is an effective election number given by

$$Z_{eff} = \int d\tau \, |\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)|^2 \times \left[\delta(\mathbf{r}_1 - \mathbf{r}_2) + \delta(\mathbf{r}_1 - \mathbf{r}_3)\right] \cdot \tag{31}$$

Z_{eff} is a measure of the probability that the positron and an atomic electron are at the same point in space.

We have used the total scattering wave function (27) with two of the different forms of ψ_0 to calculate Z_{eff}.

With the Hartree Fock function IV we get the value 3.28 for Z_{eff} and with the three term Hylleraas function III we get 3.21. These values are for the scattering wave functions obtained with S = 20. The results are presented in Table IV along with the values for Z_{eff} obtained using the wave functions with S = 4 and S = 10. Houston (1968) has previously calculated Z_{eff} using the Hartree Fock form of ψ_0 but there was an error in his computer program and the published value of 4.61 is wrong.

Drachman (1968) obtains the value 3.66 for Z_{eff} for zero energy incident positrons and these may be compared with the recent experimental value of of 3.628 ± 0.041 obtained by Lee et al. (1969) for positrons with thermal energies. Other experimental values are 3.2 (Daniel and Stump, 1959), 3.25 ± 0.22 (Duff and Heymann, 1962), 2.46 (Osmon, 1965), 3.84 (Tao and Kelly, 1969), and 3.680 ± 0.025 (Leung and Paul, 1969).

We see that our two values are very close to each other and are also in good agreement with experiment showing that our scattering wave functions are a fairly good approximation to the exact total wave function.

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TABLE I

The values of the parameters in ψ_0

	Ref.	N	Z_1	Z_2	c_1	c_2	E_0	A
I	(i)	1.529613	1.6875				-5.69531	0.99300
II	(i)	1.390139	1.8495		0.3658		-5.78224	0.99707
III	(i)	1.330518	1.81552		0.29048	0.13184	-5.80486	0.99990
IV	(ii)	0.701220	1.45580	2.91160	0.6		-5.72334	0.99598
V	(iii)	0.421074	1.571	2.5136	0.91	0.3507	-5.79613	0.99923
VI	(iv)	0.709001	2.1832	1.1886			-5.75132	0.99739

(i) Hylleraas (1929)
(ii) Green et al.(1954)
(iii) Green et al.(1958)
(iv) Shull and Löwdin(1956)

TABLE II

Scattering Lengths*

ψ_0	S = 4	10	20
I	0.061	-8.397	
II	0.052	-3.000	
III	-0.186	-0.330	-0.592
IV	-0.176	-0.309	-0.398
V	-0.143	-0.253	
VI	-0.163	-0.380	-1.341

* in units of a_0

TABLE III

The Exponential Parameters in Ψ_T

ψ_0	ε	α	β
I	2.0	0.5	0.0
II	2.0	0.5	0.0
III	3.0	0.4	-0.4
IV	4.0	0.4	-0.15
V	4.0	0.4	-0.15
VI	3.0	0.35	0.0

TABLE IV

Effective Electron Number Z_{eff}

ψ_0	S = 4	10	20
III	1.86	2.39	3.21
IV	2.06	2.48	3.28